DSSTox Log File:

NCTR Estrogen Receptor Binding Database (NCTRER)

(last updated 7 November 03)

Description: Information in this file documents the creation, review, and update process for the DSSTox NCTRER SDF files and provides summary information on database contents. The first section summarizes the process used for creating the initial DSSTox SDF files, and the quality assurance checks and procedures employed. A table providing field and data counts offers summary overview of NCTRER file contents and chemical composition. The Log table will document any future modifications and revisions to the database content or format. For the most current version of this Log File and a record of any new modifications, or to report errors in this file, a user should consult the central DSSTox website, http://www.epa.gov/nheerl/dsstox/ .

QA and Development Notes:
The DSSTox NCTRER SDF underwent an extensive series of quality review checks prior to publication of the initial launch version. The original NCTR ER database was provided by the NCTR Source (Weida Tong) in SDF format. This file contained basic chemical information (**Structure**, **CAS**, **ChemName**) and activity information **LOG ER_RBA**. We thank Weida Tong and Hong Fang for invaluable assistance in various stages of development and quality review, providing additional data fields (**LogP**), clarifying numerous issues pertaining to the experimental data, and approving all added field names and contents. Chemical structures provided by the NCTR Source in the original SDF were rendered as three dimensional (Corina, version 2.3). These 3D structures are offerred in the file NCTRER_DOP3D. For construction of the main DSSTox SDF, we redrew these structures in more easily viewed 2D form using CambridgeSoft ChemFinder (ver 7.0 for Windows). We consulted the main citation [Fang et al., 2001, Chem. Res. Tox., 14:280-294] and confirmed structures and CAS numbers at the ChemFinder website (http://chemfinder.cambridgesoft.com/). CambridgeSoft ChemFinder (ver 7.0 for Windows) was also used for automatic generation of SMILES codes from structures. There are only two chemicals classified as “organometallic” and 4 “defined organics” classified as either salt or complex in the NCTRER. The latter 4 compounds were listed in their “simplified to parent” form, i.e. in neutral or uncomplexed form, in the original NCTRER database obtained from the NCTR Source. To maintain consistency with the format of other DSSTox databases, we include the structure of the “tested form” of the 4 compounds in the main NCTRER SDF file and exclude the 2 compounds classified as “organometallic” from the NCTRER_DOP (defined organic parent) file. The NCTRER_DOP SDF file was created by exporting only defined organics to SDF from the Main ChemFinder file, and converting salts and complexes to their simplified form, with changes to corresponding Standard Chemical Fields.

Field and Data Counts in DSSTox SDF files:

DSSTox SDF	Standard Chemical Fields	Source-specific fields	Chemical records total	Defined organic	Inorganic	Organo-metallic	Mixture or unknown	Parent	Salt or Salt complex	Complex
NCTRER_v1a	14	13	232*	230	0	2	0	226	1	5
NCTRER_DOP_v1a	16	13	230*	230	0	0	0	226	1	3
NCTRER_DOP3D_v1a	16	13	230*	230	0	0	0	226	1	3

* NCTRER contains 6 sets of alpha, beta stereochemical pairs that have the same 2D representation but different 3D structures and different activities.

Chemical Counts and Activity Distribution in Main Structural Classes of NCTRER:

ChemClass	Active Strong	Active Medium	Active Weak	Slight Binder	Inactive	Total # of Chemicals	Mean ER_RBA ChemClass
Steroids	12	7	3	0	9	31	1.24
DES	13	6	2	1	0	22	2.14
Phytoestrogens	3	13	18	0	12	46	0.019
Diphenylmethanes	1	6	11	3	9	30	0.0087
Biphenyls	0	2	6	1	3	12	0.0028
Phenols	0	4	19	1	5	29	0.00088
Misc	0	3	2	2	55	62	NA
Totals	29	41	61	8	93	232	
Summed Totals	*Actives*		*131*	*Inactives*	*101*	232	

Log of SDF Modifications and Version/revision updates:

Date	DSSTox SDF File Name	Modifications from previous version	Additional Notes
23Oct03	NCTRER_v1a_232_23Oct03.sdf NCTRER_DOP_v1a_230_23Oct03.sdf NCTRER_DOP3D_v1a_230_23Oct03.sdf	Initial launch publication; no previous published versions.	NCTRER is considered a “static” historical database meaning that further expansion of the database to include additional data is unlikely. Future updates will correct reported errors provided by users or incorporate DSSTox format changes.

Wanted!! CAS Information

The Unknown CAS entries below are primarily an indication of the unstudied nature of many of the disinfection by-product entries in the DBPCAN database. However, if a user has information pertaining to any Unknown CAS in the below listing, please report this using a DSSTox Error Report Form that can be accessed from any DSSTox SDF Download Page, and be sure to indicate all relevant information (full DSSTox SDF file name, DSSTox_ID, ChemName, nature of missing information, source of correct information, etc.). Thank you!

ChemName	Structure or SMILES	CAS	SDF	Date of Request
2,3,4,5-tetrachloro-4'-biphenylol	C1(C(=C(C2C=CC(=CC=2)O)C=C(C=1Cl)Cl)Cl)Cl	Unknown	NCTRER	23Oct03
meso-p-(alpha,beta-diethyl-p-methyl-phenethyl)-phenol	C(C(C1=CC=C(C=C1)C)CC)(C2C=CC(=CC=2)O)CC	Unknown	NCTRER	23Oct03
2,6-dimethyl hexestrol	C1(C(C(C2=CC=C(O)C=C2)CC)CC)=CC(C)=C(C(=C1)C)O	Unknown	NCTRER	23Oct03
3,6,4'-trihydroxyflavone	C1(=C(OC2=CC=C(C=C(C1=O)2)O)C3=CC=C(C=C3)O)O	Unknown	NCTRER	23Oct03